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The proof on the conjecture of extremal graphs for the kth eigenvalues of trees

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Abstract

We consider the only remaining unsolved case $n \equiv 0 \pmod k$ for the largest kth eigenvalue λ_k of trees with n vertices. In this paper, the conjecture for this problem in [Shao Jia-yu, On the largest kth eignevalues of trees, Linear Algebra Appl. 221 (1995) 131–157] is proved and (from this) the complete solution to this problem, the best upper bound and the extremal trees of λ_k, is given in general cases above.

AMS classification: 05C05; 05C50

Keywords: Tree; Subtree; Characteristic polynomial; Eigenvalue

1. Introduction

Let G be a graph of order n, $A(G)$ the adjacency matrix of G, and $P(G, \lambda)$ the characteristic polynomial of $A(G)$ (sometimes $P(G, \lambda)$ is simply represented by $P(G)$). The eigenvalues of $A(G)$ are called eigenvalues of G. Now, $A(G)$ is a symmetric (0, 1) matrix, so the eigenvalues of G are all real and can be ordered as

$$\lambda_1(G) \geqslant \lambda_2(G) \geqslant \cdots \geqslant \lambda_n(G).$$

We call $\lambda_k(G)$ the kth eigenvalue of G.

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If T is a tree of order n, then T is bipartite, and its eigenvalues satisfy the relation

$$\lambda_i(T) = -\lambda_{n-i+1}(T) \quad (i = 1, 2, \ldots, n).$$

So it suffices to study those eigenvalues $\lambda_k(T)$ for $1 \leqslant k \leqslant [n/2]$. In this paper we always assume that $1 \leqslant k \leqslant [n/2]$.

There have been considerable attempts and some successes in finding the bounds for the eigenvalues of trees with n vertices. Till now, we can see the well-known sharp upper and the sharp lower bound for the largest eigenvalues [1,2], the best possible upper bound for the kth eigenvalues when $k = 2, 3, \ldots, [n/2]$ and $n \not\equiv 0 \pmod k$ [3], and the sharp lower bound for the kth positive eigenvalues when $k = 2, 3, \ldots, [n/2]$ [4].

The only remaining unsolved case is the case $n \equiv 0 \pmod k$ for the upper bound and the extremal trees of $\lambda_k(T)$. In this case, we always write $n = kt$ $(k \geqslant 2, t \geqslant 2)$.

Shao [3] showed that $\lambda_k(T) < \sqrt{t-1}$.

For further studying Shao [5] obtained the sharp upper bound of $\lambda_k(T)$ when $2 \leqslant k \leqslant 6$ and $t \geqslant 3$ $(t \neq 4)$, gave a conjecture (we will describe it latter) for the best upper bound and the extremal trees of $\lambda_k(T)$ in general case, and proved some necessary conditions when $k \geqslant 2$ and $t \geqslant 3$ $(t \neq 4)$ for this conjecture.

Also in 1991, Shao and Hong [6] gave the proof for the unsolved case $t = 2$ of the necessary condition above, and obtained the sharp bound of $\lambda_k(T)$ in that case $t = 2$ from this proof.

As a continuation, Zou et al. [7] further gave an improved necessary condition for the conjecture above.

In addition, Guo [8] lately give a sufficient and necessary condition for the upper bound of the kth eigenvalues of tree when $k = 2, \ldots, [n/2]$ and $n \not\equiv 0 \pmod k$.

In this paper this conjecture above is proved and (from this) the complete solution, the best upper bound and the extremal trees, to this only formerly unsolved problem above on $\lambda_k(T)$ is given in general cases.

To be clear, we give the same definitions as in [5,7] below.

Let $\Gamma_n = \{T, \quad T \text{ is a tree of order } n\}$,

$$\bar{\lambda}_k(n) = \max\{\lambda_k(T) | T \in \Gamma_n\} \quad (1 \leqslant k \leqslant [n/2]),$$

and $\overline{\Gamma}_{k,t} = \left\{T \in \Gamma_{kt} | \lambda_k(T) = \bar{\lambda}_k(kt)\right\}$.

The trees in $\overline{\Gamma}_{k,t}$ are called the extremal trees.

Definition 1. Let $X_{k,t}$ be the subset of trees in Γ_{kt} which consists of k disjoint stars $S_1 \cdots S_k$ of order t $(S_1 \cong S_2 \cong \cdots \cong S_k \cong K_{1,t-1})$ together with another $k-1$ edges $e_1, e_2, \ldots, e_{k-1}$ such that the two end vertices of each edge e_i $(i = 1, 2, \ldots, k-1)$ are non-central vertices of different stars. We call $S_i \cdots S_k$ the stars of this tree $T \in X_{k,t}$, call the edges $e_1, \ldots, e_{k-1}$ the non-star edges of T, and call the other edges the star edges of T.

Definition 2. Define $X'_{k,t}$ as the subset of $X_{k,t}$ which consists of those trees T in $X_{k,t}$ such that for any S_i of T, there is only one vertex in S_i incident to some non-star edges of T.

Conjecture [5]. *For $t \geqslant 2$, we have*

$$\overline{\Gamma}_{k,t} = \{T^*_{k,t}\} \quad \textit{and} \quad \bar{\lambda}_k(kt) = \sqrt{t - 1 + \lambda_2(f(y))},$$

where $\lambda_2(f(y))$ is the second largest root of the equation

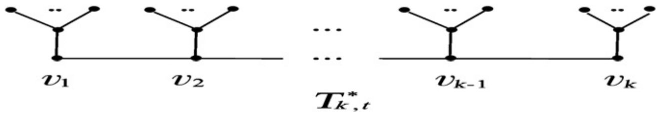

Fig. 1. The extremal tree in the conjecture [5].

$$f(y) = y^2(y + t - 1) - 4(y + 1)^2 \cos^2 \frac{\pi}{k + 1} = 0$$

and $\{T^*_{k,t}\}$ *is the tree in Fig.* 1.

Let $T \in X_{k,t}$. If there is only one non-star edge uv incident to a star S_i of T (say $v \in V(S_i)$), we will call the vertex v the pendant star vertex of T. For example, these vertices v_1 and v_k in Fig. 1.

If T_1 is a subtree of $T \in X_{k,t}$ and the vertex set $V(T_1) = V(S_{i_1}) \dot\cup \cdots \dot\cup V(S_{i_l})$ where $S_{i_j} \in \{S_1, \ldots, S_k\}$, obviously, $T_1 \in T_{l,t}$. In the following, we usually denote such a subtree T_1 by $T_{l,t}$.

2. Lemmas and conclusions

Lemma 1 [2]. *Let u and v be the adjacency vertices in a forest F. Then*

$$P(F, \lambda) = P(F - uv, \lambda) - P(F - u - v, \lambda).$$

Lemma 2 [3]. *Let G be a graph. Then*

$$\lambda_i(G) \geqslant \lambda_i(G - V') \geqslant \lambda_{i+k}(G) \quad \textit{for } V' \subset V(T) \textit{ and } |V'| = k.$$

Lemma 3 [3]. *Let F be a forest with n vertices. Then*

$$\lambda_k(F) \leqslant \sqrt{\left[\frac{n}{k}\right] - 1} \quad \left(1 \leqslant k \leqslant \left[\frac{n}{2}\right]\right).$$

Lemma 4 [5].

(1) *For* $k \geqslant 1$ *and* $t \geqslant 2$, *we have*

$$\lambda_k(T^*_{k,t}) = \sqrt{t - 1 + \lambda(f(y))} \quad \textit{and} \quad \lambda_k(T^*_{k,t}) > \lambda_{k+1}(T^*_{k+1,t}),$$

where $f(y) = y^2(y + t - 1) - 4(y + 1)^2 \cos^2 \frac{\pi}{k+1}$ *and* $\lambda(f(y))$ *is the unique root of* $f(y)$ *on the interval* $(-1, 0]$.

(2) *For* $k \geqslant 2$ *and* $t \geqslant 2$, *we have*

$$\lambda_k(T) < \lambda_k(T^*_{k,t}) \quad \textit{for } T \in X'_{k,t} \backslash \{T^*_{k,t}\}.$$

Lemma 5 [5, 6]. *For* $k \geqslant 2$ *and* $t \geqslant 2$ $(t \neq 4)$, *we have*

$$\lambda_k(T) < \lambda_k(T^*_{k,t}) \quad (T \in \Gamma_{kt} \backslash X_{k,t}) \qquad \textit{i.e. } \overline{\Gamma}_{k,t} \subseteq X_{k,t}.$$

Lemma 6. *Let* $T \in X_{k,t}$. *For any subtree* $T_{l,t}$ *of* T $(1 \leqslant l \leqslant k - 1)$, *there exists a vertex subset* $V' \subset V(T)$, $|V'| = k - l$, *such that*

$$T - V' = T_{l,t} \dot\cup \underbrace{K_{1,t-2} \dot\cup \cdots \dot\cup K_{1,t-2}}_{k-l}.$$

Proof. Obviously this conclusion holds for $k = 2$. For $k \geqslant 3$ we use induction on k.

Case I: $l \leqslant k - 2$. For $T_{l,t}$ it is evident that there exists one pendant star vertex $v \in V(T)$ and $v \notin V(T_{l,t})$ (otherwise, for any $S_i \notin T_{l,t}$, there are at least two non-star edges incident to S_i. Then there is the cycle in T). Thus we have

$$T - v = T_{k-1,t} \dot{\cup} K_{1,t-2},$$

where $T_{k-1,t} \in X_{k-1,t}$, $v \notin T(T_{k-1,t})$, and $T_{l,t}$ is a subtree of $T_{k-1,t}$.
By induction we also have there are vertices $v_1 \cdots v_{k-1-l} \in V(T_{k-1,t})$ such that

$$T_{k-1,t} - \{v_1, \ldots, v_{k-1-l}\} = T_{l,t} \dot{\cup} \underbrace{k_{1,t-2} \dot{\cup} \cdots \dot{\cup} k_{1,t-2}}_{k-1-l}.$$

Thus

$$T - \{v_1, \ldots, v_{k-1-l}, v\} = T_{l,t} \dot{\cup} \underbrace{K_{1,t-2} \dot{\cup} \cdots \dot{\cup} K_{1,t-2}}_{k-l}.$$

Case II: $l = k - 1$. For $T_{k-1,t}$ there exists one pendant star vertex $v \notin T_{k-1,t}$ in T (otherwise, there is the cycle in T). So this conclusion comes from that

$$T - v = T_{k-1,t} \dot{\cup} K_{1,t-2}. \qquad \square$$

Corollary 6.1. *Let $T \in X_{k,t}$. Then for any subtree $T_{l,t}$ of T $(1 \leqslant l \leqslant k - 1)$, we have that for $\lambda_k(T)$*

$$\sqrt{t-2} < \lambda_k(T) \leqslant \lambda_l(T_{l,t}).$$

Proof. Taking $T_{l,t} = T_{1,t}$ and $V' \subset V(T)$ in Lemma 6 and using Lemma 2, we have

$$\lambda_k(T) \geqslant \lambda_k(T - V') = \lambda_k(K_{1,t-1} \dot{\cup} K_{1,t-2} \dot{\cup} \cdots \dot{\cup} K_{1,t-2}) = \sqrt{t-2}.$$

Then, taking $T_{l,t}$ and $V'' \subset V(T)$ in Lemma 6, and by Lemma 2 and inequality above

$$\lambda_k(T) \leqslant \lambda_l(T - V'') = \lambda_l(T_{l,t} \dot{\cup} K_{1,t-2} \dot{\cup} \cdots \dot{\cup} K_{1,t-2}) = \lambda_l(T_{l,t}).$$

Now, we only need to prove that $\lambda_k(T) \neq \sqrt{t-2}$. In case $t = 2$ we have $\lambda_k(T) > \sqrt{2-2}$ by the size of maximum matching of T is k. Let $t \geqslant 3$ below.

For $k = 2$, taking the pendant star vertex v in S_1 and the central vertex $u \in S_1$, then we have from Lemma 1 that (where T_1 is some subtree of T)

$$P(T) = P(K_{1,t-2} \dot{\cup} T_1) - P(K_{1,t-1} \dot{\cup} K_{1,0} \dot{\cup} \cdots \dot{\cup} K_{1,0}).$$

Thus

$$P(T, \sqrt{t-2}) \neq 0.$$

For $k \geqslant 3$, there exists a pendant star vertex v (say $v \in S_1$). Otherwise, there is the cycle in T. So taking the vertex v and the central vertex $u \in S_1$ in Lemma 1, we have

$$P(T) = P(K_{1,t-2} \dot{\cup} T_1) - P(T_2 \dot{\cup} K_{1,0} \dot{\cup} \cdots \dot{\cup} K_{1,0}),$$

where T_1 is some subtree of T and $T_2 \in X_{k-1,t}$.

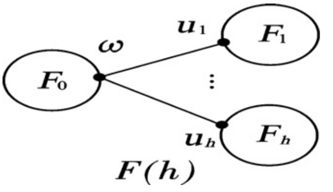

Fig. 2. The forest $F(h)$ in the Lemma 7.

And by induction we also have

$$P(T_2, \sqrt{t-2}) \neq 0.$$

Thus

$$P(T, \sqrt{t-2}) \neq 0. \qquad \square$$

We can obtain some better upper bounds than the known upper bound $\sqrt{t-1}$ in [3] from Corollary 6.1 here. But we want to do the best.

Lemma 7. *Let $F(h)$ be a forest formed by drawing h new forests $F_1, F_2, \ldots, F_h$ from a vertex ω in a forest F_0 (shown in Fig. 2). It follows that for $h \geqslant 1$*

$$P(F(h), \lambda) = P\left(\dot{\bigcup_{0 \leqslant i \leqslant h}} F_i, \lambda\right) - \sum_{i=1}^{h} P\left((F_0 - \omega) \,\dot{\cup}\, (F_i - u_i) \dot{\bigcup_{\substack{1 \leqslant j \leqslant h \\ j \neq i}}} F_j, \lambda\right).$$

Proof. For $h = 1$, taking $uv = \omega u_1$ in Lemma 1, we have

$$P(F(1)) = P(F_0 \,\dot{\cup}\, F_1) - P((F_0 - \omega) \,\dot{\cup}\, (F_1 - u_1)).$$

For $h \geqslant 2$, (we use induction on h) taking $uv = \omega u_h$ in Lemma 1,

$$P(F(h)) = P(F(h-1) \,\dot{\cup}\, F_h) - P\left((F_0 - \omega) \,\dot{\cup}\, (F_h - u_h) \,\dot{\cup} \left(\dot{\bigcup_{1 \leqslant j \leqslant h-1}} F_j\right)\right).$$

So we have by induction that

$$P(F(h)) = P(F_h)\left(P\left(\dot{\bigcup_{0 \leqslant i \leqslant h-1}} F_i\right) - \sum_{i=1}^{h-1} P\left((F_o - \omega) \,\dot{\cup}\, (F_i - u_i) \,\dot{\cup} \left(\dot{\bigcup_{\substack{1 \leqslant j \leqslant h-1 \\ j \neq i}}} F_j\right)\right)\right)$$
$$- P\left((F_0 - \omega) \,\dot{\cup}\, (F_h - u_h) \,\dot{\cup} \left(\dot{\bigcup_{1 \leqslant j \leqslant h-1}} F_j\right)\right). \qquad \square$$

Let $T \in X_{k,t}$, and S_i be a star of T with the central vertex ω_0, while ω_1 and ω_2 are two non-central vertices of the star S_i. Let $T_1, \ldots, T_h$ be the connected components of the graph $T - \omega_1$ which do not contain the vertex ω_0, and $T_1', \ldots, T_l'$ be the connected components of $T - \omega_2$ which do not contain the vertex ω_0. Finally, let T_1'' be the graph obtained from T by deleting all the vertices in $T_1, \ldots, T_h$ and $T_1', \ldots, T_l'$. Then by the comment made at the end of Section 1 we can see that there exist integers $k_1, \ldots, k_h$ and $k_1', \ldots, k_l'$ and k'' with their sum equal to k such that

$$T_i \in X_{k_i,t}, T_j' \in X_{k_j',t} \quad \text{and} \quad T_1'' \in X_{k'',t}.$$

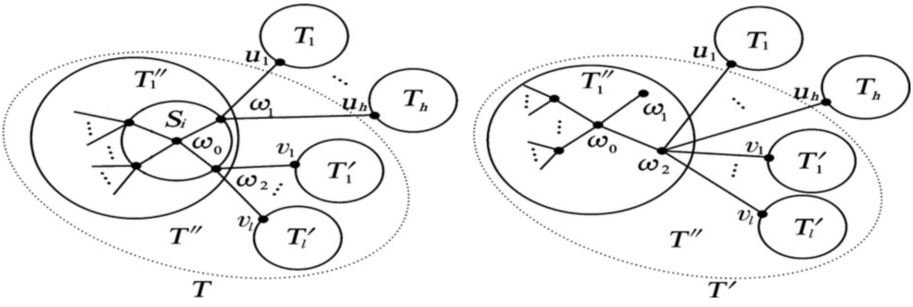

Fig. 3. The tree T and T' in the Lemma 8.

Furthermore, let

$$T' = T - \omega_1 u_1 - \cdots \omega_1 u_h + \omega_2 u_1 + \cdots + \omega_2 u_h.$$

Then we can easily see that $T' \in X_{k,t}$, and they can be shown in Fig. 3.

Lemma 8. *Let $T \in X_{k,t}$ (T and T' are shown in Fig. 3). Then $T' \in X_{k,t}$ and we have that for $k \geqslant 3, t \geqslant 3, h \geqslant 1,$ and $l \geqslant 1$*

(1) $P(T,\lambda) = P(T',\lambda) + \sum\limits_{1\leqslant i\leqslant h} \sum\limits_{1\leqslant j\leqslant l} P(F_{i,j},\lambda),$

where $F_{i,j} = (T_1'' - \omega_1 - \omega_2) \dot{\cup} (T_i - u_i) \dot{\cup} (T_j' - u_j) \dot{\cup} \left(\dot{\bigcup}_{\substack{1\leqslant s\leqslant h \\ s\neq i}} T_s \right) \dot{\cup} \left(\dot{\bigcup}_{\substack{1\leqslant p\leqslant l \\ p\neq j}} T_p' \right).$

(2) $\lambda_{k-2}(F_{i,j}) \leqslant \lambda_k(T') \leqslant \lambda_{k-3}(F_{i,j}),$

where we agree that $\lambda_0(F_{i,j}) = +\infty.$

Proof. For T and T' we may write $T_i \in X_{k_i,t}$, $T_j' \in X_{k_j',t}$, and $T_1'' \in X_{k'',t}$.

Taking $F_0 = T''$ and $F_0 = T'' - \omega_1$ in Lemma 7, then

$$P(T') = P\left(T'' \dot{\cup} \left(\dot{\bigcup}_{1\leqslant i\leqslant h} T_i\right)\right) - \sum_{i=1}^{h} P\left((T'' - \omega_2) \dot{\cup} (T_i - u_i) \dot{\cup} \left(\dot{\bigcup}_{\substack{1\leqslant s\leqslant h \\ s\neq i}} T_s\right)\right).$$

$$\begin{aligned} P(T) &= P\left(T'' \dot{\cup} \left(\dot{\bigcup}_{1\leqslant i\leqslant h} T_i\right)\right) - \sum_{i=1}^{h} P\left((T'' - \omega_1) \dot{\cup} (T_i - u_i) \dot{\cup} \left(\dot{\bigcup}_{\substack{1\leqslant s\leqslant h \\ s\neq i}} T_s\right)\right) \\ &= P\left(T'' \dot{\cup} \left(\dot{\bigcup}_{1\leqslant i\leqslant h} T_i\right)\right) - \sum_{i=1}^{h} P\left((T_i - u_i) \dot{\cup} \left(\dot{\bigcup}_{\substack{1\leqslant s\leqslant h \\ s\neq i}} T_s\right)\right) \\ &\quad \times \Bigg[P\left((T_1'' - \omega_1) \dot{\cup} \left(\dot{\cup}_{1\leqslant j\leqslant l} T_j'\right)\right) \\ &\quad - \sum_{j=1}^{l} P\left((T_1'' - \omega_1 - \omega_2) \dot{\cup} (T_j' - v_j) \dot{\cup} \left(\dot{\bigcup}_{\substack{1\leqslant p\leqslant L \\ p\neq j}} T_p'\right)\right)\Bigg]. \end{aligned}$$

So, noticing that $(T''-\omega_2)\cong\left((T_1''-\omega_1)\,\dot{\cup}\,(\dot{\cup}_{1\leqslant j\leqslant l}T_j')\right)$, we have

$$P(T)=P(T')+\sum_{\substack{1\leqslant i\leqslant h\\1\leqslant j\leqslant l}}P\left((T_1''-\omega_1-\omega_2)\,\dot{\cup}\,(T_i-u_i)\right.$$
$$\left.\dot{\cup}\,(T_j'-v_j)\,\dot{\cup}\left(\dot{\bigcup_{\substack{1\leqslant s\leqslant h\\s\neq i}}}T_s\right)\dot{\cup}\left(\dot{\bigcup_{\substack{1\leqslant p\leqslant l\\p\neq j}}}T_p'\right)\right). \quad (1)$$

This proves conclusion (1).

Moreover, by Lemma 3

$$\begin{aligned}
&\lambda_{k_s+1}(T_s)\leqslant\sqrt{\left[\frac{k_st}{k_s+1}\right]-1}\leqslant\sqrt{t-2},\\
&\lambda_{k_p'+1}(T_p')\leqslant\sqrt{t-2},\\
&\lambda_{k_i}(T_i-u_i)\leqslant\sqrt{\left[\frac{k_it-1}{k_i}\right]-1}=\sqrt{t-2},\\
&\lambda_{k_j'}(T_j'-v_j)\leqslant\sqrt{t-2},\\
&\lambda_{k''}(T_1''-\omega_1-\omega_2)\leqslant\sqrt{t-2}
\end{aligned} \quad (2)$$

also, by Corollary 6.1

$$\lambda_k(T')\geqslant\sqrt{t-2} \quad (3)$$

and also, by Corollary 6.1 and Lemma 2 (We agree that $\lambda_0(G)=+\infty$ for a graph G.)

$$\begin{aligned}
&\lambda_k(T')\leqslant\lambda_{k_s}(T_s),\\
&\lambda_k(T')\leqslant\lambda_{k_p'}(T_p'),\\
&\lambda_k(T')\leqslant\lambda_{k_i}(T_i)\leqslant\lambda_{k_i-1}(T_i-u_i),\\
&\lambda_k(T')\leqslant\lambda_{k_j'}(T_j')\leqslant\lambda_{k_j'-1}(T_j'-v_j),\\
&\lambda_k(T')\leqslant\lambda_{k''}(T_1'')\leqslant\lambda_{k''-1}(T_1''-\omega_0)=\lambda_{k''-1}((T_1''-\omega_0-\omega_1-\omega_2)\,\dot{\cup}\,k_{1,0}\,\dot{\cup}\,k_{1,0})\\
&\qquad=\lambda_{k''-1}(T_1''-\omega_0-\omega_1-\omega_2)\leqslant\lambda_{k''-1}(T_1''-\omega_1-\omega_2).
\end{aligned} \quad (4)$$

Thus we have from (2)–(4) that for $\lambda_k(T')$

$$\begin{aligned}
&\lambda_{k_s+1}(T_s)\leqslant\lambda_k(T')\leqslant\lambda_{k_s}(T_s),\\
&\lambda_{k_p'+1}(T_p')\leqslant\lambda_k(T')\leqslant\lambda_{k_p'}(T_p'),\\
&\lambda_{k_i}(T_i-u_i)\leqslant\lambda_k(T')\leqslant\lambda_{k_i-1}(T_i-u_i),\\
&\lambda_{k_j'}(T_j'-v_j)\leqslant\lambda_k(T')\leqslant\lambda_{k_j'-1}(T_j'-v_j),\\
&\lambda_{k''}(T_1''-\omega_1-\omega_2)\leqslant\lambda_k(T')\leqslant\lambda_{k''-1}(T_1''-\omega_1-\omega_2)
\end{aligned} \quad (5)$$

and thus, noticing that $(k_i-1)+(k_j'-1)+(k''-1)+\sum_{\substack{1\leqslant s\leqslant h\\s\neq i}}k_s+\sum_{\substack{1\leqslant p\leqslant l\\p\neq j}}k_p'=k-3$, it follows that

$$\lambda_{k-2}(F_{i,j}) \leqslant \lambda_k(T') \leqslant \lambda_{k-3}(F_{i,j}). \tag{6}$$

It can be checked that the inequality (6) holds when there are some numbers which are equal to 1 among k_i, k'_j and k'' (the inequality (6) is that $\lambda_{k-2}(F_{i,j}) \leqslant \lambda_k(T')$ when $k = 3$). Thus conclusion (2) is proved. □

The following Theorem 1 will show that the kth eigenvalues become greater as making such transformations (in Fig. 3) of the structure of the tree in $X_{k,t}$.

Theorem 1. *Let $T \in X_{k,t}$. Then $T' \in X_{k,t}$ (T and T' are shown in Fig. 3) and we have that for $k \geqslant 3, t \geqslant 3, h \geqslant 1$, and $l \geqslant 1$*

$$\lambda_k(T) \leqslant \lambda_k(T').$$

Proof. Suppose to the contrary that

$$\lambda_k(T) > \lambda_k(T').$$

Then we have from Lemma 3 and Corollary 6.1 that for $\lambda_k(T')$

$$\lambda_{k+1}(T) \leqslant \sqrt{\left[\frac{kt}{k+1}\right] - 1} \leqslant \sqrt{t-2} < \lambda_k(T') < \lambda_k(T).$$

It follows that

$$(-1)^k P(T, \lambda_k(T')) = (-1)^k \prod_{1\leqslant i\leqslant n} (\lambda_k(T') - \lambda_k(T)) > 0.$$

On the other hand, we also have by Lemma 8 (2) that (for any i and j)

$$(-1)^k P(F_{i,j}, \lambda_k(T')) \leqslant 0.$$

So by Lemma 8 (1) we have

$$(-1)^k P(T, \lambda_k(T')) = \sum_{1\leqslant i\leqslant h} \sum_{1\leqslant j\leqslant l} (-1)^k P(F_{i,j}, \lambda_k(T')) \leqslant 0.$$

A contradiction. □

The following Theorem 2 will prove that Shao's conjecture is true and, thus, give the complete solution to the only formerly unsolved problem of $\lambda_k(T)$ in general cases.

Theorem 2. *For $k \geqslant 1$ and $t \geqslant 2$ ($t \neq 4$), we have*

$$\overline{\Gamma}_{k,t} = \{T^*_{k,t}\}$$

and

$$\bar{\lambda}_k(kt) = \lambda_k(T^*_{k,t}) = \sqrt{t - 1 + \lambda(f(y))},$$

where $\lambda(f)$ is the unique root to the equation $f(y) = y^2(y + t - 1) - 4(y + 1)^2 \cos^2 \frac{\pi}{k+1} = 0$ on the interval $(-1, 0]$.

Proof. For $k = 1$, the conclusion is just the well-known sharp upper bound of $\lambda_1(T)$. In case $k = 2$ we have $\overline{\Gamma}_{2,t} = \{T^*_{2,t}\}$ from $X_{2,t} = \{T^*_{2,t}\}$ and Lemma 5, and in case $t = 2$ $\overline{\Gamma}_{k,2} = \{T^*_{k,2}\}$

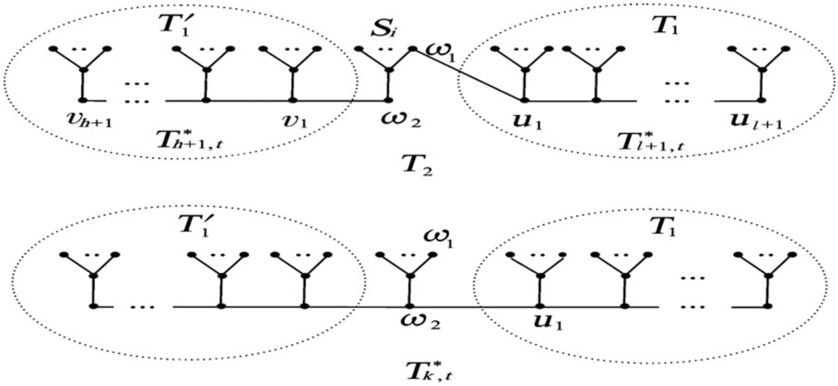

Fig. 4. The trees in the inequality (2).

from $X_{k,2} = X'_{k,2}$ and Lemmas 4 and 5. So we will consider general cases $k \geqslant 3$ and $t \geqslant 3$. Let $T \in X_{k,t}$ and $T \ncong T^*_{k,t}$ below.

Case I: There is one star S_{i_0} of T incident to at least three non-star edges of T.

We apply Theorem 1 repeatedly to every star S_i of T, and transform T into a tree T_1 in $X_{k,t}$ in which for any star S_i of T_1 there is only one vertex (it is non-central vertex) in S_i incident to some non-star edges of T_1.

Notice that there are at least three non-star edges of T_1 incident to S_{i_0}, thus $T_1 \in X'_{k,t}$ and $T_1 \ncong T^*_{k,t}$, and therefore we have from Theorem 1 and Lemma 4(2) that

$$\lambda_k(T) \leqslant \lambda_k(T_1) < \lambda_k(T^*_{k,t}). \tag{1}$$

Case II: For any star S_i of T, S_i incident to at most two non-star edges of T.

By applying some transforms as in Case I, we can transform T into the tree T_2, which is shown in Fig. 4 (we can obtain the best possible upper bound of $\lambda_k(T)$ by transforming T into $T^*_{k,t}$ directly. But we want to do better).

Now, by Theorem 1

$$\lambda_k(T) \leqslant \lambda_k(T_2) \leqslant \lambda_k(T^*_{k,t}). \tag{2}$$

So we only need to prove that $\lambda_k(T_2) \neq \lambda_k(T^*_{k,t})$.

From Lemma 8 (1)

$$P(T^*_{k,t}) = P(T_2) - P((S_i - \omega_1 - \omega_2) \dot{\cup} (T_1 - u_1) \dot{\cup} (T_1' - v_1)),$$

where $T_1 - u_1 \cong T^*_{l,t} \dot{\cup} K_{1,t-2}$, $T_1' - v_1 \cong T^*_{h,t} \dot{\cup} k_{1,t-2}$, and $S_i - \omega_1 - \omega_2 \cong K_{1,t-3}$ ($h \geqslant 0$, $l \geqslant 0$, and we agree $T^*_{0,t} \dot{\cup} G = G$).

So, let $F = T^*_{h,t} \dot{\cup} T^*_{l,t} \dot{\cup} k_{1,t-3} \dot{\cup} k_{1,t-2} \dot{\cup} k_{1,t-2}$. Then

$$P(T^*_{k,t}) = P(T_2) - P(F). \tag{3}$$

On the other hand, by Lemma 4(1)

$$\begin{aligned} &\lambda_1(K_{1,t-3}) \leqslant \sqrt{t-2} < \lambda_k(T^*_{k,t}), \\ &\lambda_1(K_{1,t-2}) = \sqrt{t-2} < \lambda_k(T^*_{k,t}). \end{aligned} \tag{4}$$

And by Lemma 3 and Lemma 4(1)

$$\begin{aligned}&\lambda_{h+1}(T^*_{h,t}) \leqslant \sqrt{t-2} < \lambda_k(T^*_{k,t}) < \lambda_h(T^*_{h,t}) \quad (h \geqslant 1),\\ &\lambda_{l+1}(T^*_{l.t}) \leqslant \sqrt{t-2} < \lambda_k(T^*_{k,t}) < \lambda_l(T^*_{l,t}) \quad (l \geqslant 1).\end{aligned} \tag{5}$$

So from (4) and (5) we have

$$P(F, \lambda_k(T^*_{k,t})) \neq 0. \tag{6}$$

It can be checked that the inequality (6) still holds when $h = 0$ or $l = 0$ or $h = l = 0$.

Thus we obtain by (3) and (6) that

$$P(T_2, \lambda_k(T^*_{k,t})) = P(F, \lambda_k(T^*_{k,t})) \neq 0.$$

These prove conclusion. □

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